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SUBJECT: A Simple Method for Approximating Quantiles of the Random Variable $X_1^2 + X_2^2 + X_3^2$ - Case 310

DATE: August 9, 1968

FROM: H. J. Bixhorn
B. G. Niedfeldt

ABSTRACT

Two approaches are taken to study the distribution of the expression $X_1^2 + X_2^2 + X_3^2$ where the X_i are mutually independent random variables distributed as $N(0,\sigma_i^2)$ $(i=1,2,3)$. First, a simple method is given to find ζ_p, an approximation for the quantile of order p, i.e., given $0 < p < 1$, ζ_p will be found such that $P\{X_1^2 + X_2^2 + X_3^2 \leq \zeta_p\} \simeq p$. A more complex, exact method for determining $P\{X_1^2 + X_2^2 + X_3^2 \leq r^2\}$ given any $r > 0$ is then discussed. This method is used to demonstrate the accuracy of the approximation, ζ_p.

Both methods can be applied to any correlated normal random vector by performing a proper orthogonal transformation to diagonalize the covariance matrix. The first method, however, has the advantage that all necessary information can be obtained from the original covariance matrix without diagonalization.

Although the discussion and examples presented here deal only with the expression $X_1^2 + X_2^2 + X_3^2$, the techniques can easily be extended to any quadratic form $a_1 X_1^2 + a_2 X_2^2 + a_3 X_3^2$.

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MEMORANDUM FOR FILE

INTRODUCTION

Given a set of three independent, normally distributed random variables with $EX_i = 0$, Var $X_i = \sigma_i^2$ $(i=1,2,3)$, it is known that $X_1^2/\sigma_1^2 + X_2^2/\sigma_2^2 + X_3^2/\sigma_3^2$ has a χ_3^2-distribution. If $\sigma_1^2 = \sigma_2^2 = \sigma_3^2$, $(X_1^2 + X_2^2 + X_3^2)/\sigma_1^2$ is distributed as χ_3^2 or, equivalently, $X_1^2 + X_2^2 + X_3^2$ is a $\sigma_1^2\chi_3^2$-variate. For the general case where the variances are not equal, the assumption was made that by an appropriate choice of σ^2 and ν, $X_1^2 + X_2^2 + X_3^2$ could be approximated by a $\sigma^2\chi_\nu^2$-variate. Here ν is not necessarily an integer.

NOTE: It should be recalled that the χ_n^2-distribution (n is an integer) is a special case of the gamma distribution. The density of a random variable obeying a gamma distribution is given by

$$f(x) = \begin{cases} 0 & x \leq 0 \\ \dfrac{b^q}{\Gamma(q)} x^{q-1} e^{-bx} & x > 0 \end{cases}$$

when $b > 0$, $q > 0$. When $b = \frac{1}{2\sigma^2}$ and $q = \frac{n}{2}$ for positive integer n, the random variable is said to have a χ_n^2-distribution. By taking $q = \frac{\nu}{2}$ where ν is positive but not necessarily an integer, the notion of a χ^2-distribution can be extended to cover the case of non-integer degrees of freedom.

Once σ^2 and ν are determined, the distribution of a $\sigma^2 \chi_\nu^2$-variate can be used to find ζ_p for any $0 < p < 1$ such that

$$P\{X_1^2 + X_2^2 + X_3^2 \leq \zeta_p\} \simeq p \quad .$$

In section 2, an exact method developed by Grad and Solomon [1], which is based on use of the Laplace transform, is shown to give $P\{X_1^2 + X_2^2 + X_3^2 \leq r^2\}$ for any $r > 0$. This method can be used to check the accuracy of ζ_p found in section 1 by setting $r^2 = \zeta_p$ in order to calculate the exact value of $P\{X_1^2 + X_2^2 + X_3^2 \leq \zeta_p\}$.

The study of the distribution of quadratic forms has been approached from various other points of view. A very obvious way of determining $P\{X_1^2 + X_2^2 + X_3^2 \leq r^2\}$ results from treating this as the probability that the 3-dimensional normal random vector (X_1,X_2,X_3) lies in a sphere of radius r, centered at the origin. Thus

$$P\{X_1^2 + X_2^2 + X_3^2 \leq r^2\} = \iiint_{x_1^2+x_2^2+x_3^2 \leq r^2} f(x_1,x_2,x_3)dx_1 \, dx_2 \, dx_3$$

where $f(x_1,x_2,x_3)$ is the trivariate normal density function. This development was taken by Harter [2] and Weingarten and DiDonato [3] for the 2-dimensional case. It was considered for the present problem, but the relative ease of obtaining numerical results by Grad and Solomon ruled this out.

Other papers related to the distribution of quadratic forms are listed in the references. Of particular interest is the paper by Ruben [4], which includes a recursive relationship for determining $P\left\{\sum_{i=1}^{N} X_i^2 \leq r^2\right\}$ if $P\left\{\sum_{i=1}^{N-1} X_i^2 \leq r^2\right\}$ is known (see section 7, page 613).

1. Approximation Of $X_1^2 + X_2^2 + X_3^2$ by a $\sigma^2\chi_\nu^2$-Variate

Consider the expression $X_1^2 + X_2^2 + X_3^2$ where the X_i's are independently distributed as $N(0,\sigma_i^2)$ $(i=1,2,3)$. If $\sigma_1^2 = \sigma_2^2 = \sigma_3^2$, then $(X_1^2 + X_2^2 + X_3^2)/\sigma_1^2$ is a χ_3^2-variate. If $\sigma_1^2 > 0$, $\sigma_2^2 = \sigma_3^2 = 0$, then X_2 and X_3 are constant and $(X_1^2 + X_2^2 + X_3^2)/\sigma_1^2$ is a χ_1^2-variate. Similarly if $\sigma_1^2 > 0$, $\sigma_2^2 = \sigma_1^2$, $\sigma_3^2 = 0$ or $\sigma_1^2 > 0$, $\sigma_2^2 = 0$, $\sigma_3^2 = \sigma_1^2$, then $(X_1^2 + X_2^2 + X_3^2)/\sigma_1^2$ is a χ_2^2-variate. From this it would seem that as the value of each of the variances σ_2^2 and σ_3^2 increases from 0 to σ_1^2, $(X_1^2 + X_2^2 + X_3^2)/\sigma_1^2$ may be approximated by a χ_ν^2-variate with ν increasing from 1 to 3. For values of σ_2^2 and σ_3^2 between 0 and σ_1^2, the following expression was considered for ν:

$$\nu = 1 + \frac{\sigma_2^2}{\sigma_1^2} + \frac{\sigma_3^2}{\sigma_1^2} \qquad (\sigma_1^2 \text{ was assumed to be the largest variance})$$

This equation for ν satisfies the above conditions, but other expressions satisfying these conditions could also have been considered. It happens, however, that this equation is the same as that obtained by equating the first moment of $X_1^2 + X_2^2 + X_3^2$ to that of $\sigma_1^2\chi_\nu^2$:

$$E(X_1^2 + X_2^2 + X_3^2) = E(\sigma_1^2\chi_\nu^2)$$

$$\sigma_1^2 + \sigma_2^2 + \sigma_3^2 = \sigma_1^2\,\nu$$

$$\nu = 1 + \frac{\sigma_2^2}{\sigma_1^2} + \frac{\sigma_3^2}{\sigma_1^2} \quad .$$

This provided motivation to consider the first two moments of $X_1^2 + X_2^2 + X_3^2$ in order to obtain a better approximation. Thus σ_1^2 was replaced by a constant, say σ^2, which with ν was determined by equating the first two moments of $X_1^2 + X_2^2 + X_3^2$ to those of a $\sigma^2\chi_\nu^2$-variate.

$$E(X_1^2 + X_2^2 + X_3^2) = E(\sigma^2\chi_\nu^2) \tag{1}$$

$$\mathrm{Var}(X_1^2 + X_2^2 + X_3^2) = \mathrm{Var}(\sigma^2\chi_\nu^2) \tag{2}$$

(1) becomes $\sigma_1^2 + \sigma_2^2 + \sigma_3^2 = \sigma^2\nu$ and (2) is $2(\sigma_1^4 + \sigma_2^4 + \sigma_3^4) = 2\sigma^4\nu$. Hence,

$$\sigma^2 = \frac{\sigma_1^4 + \sigma_2^4 + \sigma_3^4}{\sigma_1^2 + \sigma_2^2 + \sigma_3^2} \tag{3}$$

$$\nu = \frac{(\sigma_1^2 + \sigma_2^2 + \sigma_3^2)^2}{\sigma_1^4 + \sigma_2^4 + \sigma_3^4} \tag{4}$$

Because ν is generally not an integer, the value of $\zeta_p(\nu)$ such that $P\{\sigma^2\chi_\nu^2 \leq \zeta_p(\nu)\} = p$ is not available from tables of the χ^2-distribution. Three-point interpolation through the points $(\nu, \zeta_p(\nu)/\sigma^2)(\nu=1,2,3)$ was used to find this value. Then under the assumption that $X_1^2 + X_2^2 + X_3^2$ can be approximated by a $\sigma^2\chi_\nu^2$-variate, we have

$$P\{X_1^2 + X_2^2 + X_3^2 \leq \zeta_p(\nu)\} \simeq p \quad \text{for any} \quad 0 < p < 1 .$$

The practice of approximating the distribution of a quadratic form by a χ^2-distribution using the above method is in widespread use. Grad and Solomon refer to this method and give a limited number of examples using it.

2. Exact Distribution of $X_1^2 + X_2^2 + X_3^2$ by Characteristic Functions

In working with sums of independent random variables, common use is made of characteristic functions to determine the distribution of the sum. The characteristic function of a random variable with probability density f(x) is defined by

$$\phi(s) = \int_{-\infty}^{\infty} e^{isx} f(x)dx \qquad (-\infty < s < \infty)$$

and the inverse transformation is given by

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-isx} \phi(s)ds$$

Now the characteristic function of a random variable X^2 such that X is $N(0,\sigma^2)$ is $(1-2\sigma^2 is)^{-1/2}$. Consider the random variable $X_1^2 + X_2^2 + X_3^2$ where the X_j are mutually independent and $N(0,\sigma_j^2)$ (j=1,2,3). Because the characteristic function of a sum of independent random variables is the product of the characteristic functions of the individual random variables, the characteristic function of $X_1^2 + X_2^2 + X_3^2$ is given by

$$\prod_{j=1}^{3} (1 - 2\sigma_j^2 is)^{-1/2} .$$

Grad and Solomon arrive at a form for the inverse transformation of this characteristic function which is suitable for computational purposes. In the course of the derivation, the variances are normalized by dividing each by $\sum_1^3 \sigma_i^2$. Thus the density f(t) and the distribution function F(t) given in Grad-Solomon refer to the random variable $(X_1^2 + X_2^2 + X_3^2)/\sum_1^3 \sigma_i^2$. Thus if g(t) and G(t) are the density and distribution functions of $X_1^2 + X_2^2 + X_3^2$, then

$$g(t) = \frac{1}{\Sigma \sigma_i^2} f\left(\frac{t}{\Sigma \sigma_i^2}\right) \tag{5}$$

$$G(t) = F\left(\frac{t}{\Sigma \sigma_i^2}\right) \quad . \tag{6}$$

There appears to be a minor error in the equations Grad-Solomon give for f(t) and F(t) in the case of unequal variances. Equations (12) and (15) in Grad-Solomon do not yield (25) and (26). Apparently there was a mix-up in the constants c_1, c_2, c_3. This was corrected to give equations (7) and (8) of this memorandum.

<u>$\sigma_1^2 < \sigma_2^2 < \sigma_3^2$</u>

$$f(t) = \frac{1}{\pi}\sqrt{\frac{c_1 c_2 c_3}{2}}\, e^{-\frac{1}{4}(c_2+c_3)t} \int_{-1}^{1} \frac{e^{\frac{1}{4}(c_2-c_3)tx}}{\sqrt{2c_1-(c_2+c_3)+(c_2-c_3)x}} \cdot \frac{dx}{\sqrt{1-x^2}} + r(t) \tag{7}$$

$$F(t) = 1 - \frac{1}{\pi}\sqrt{8c_1 c_2 c_3}\, e^{-\frac{1}{4}(c_2+c_3)t} \cdot \int_{-1}^{1} \frac{e^{\frac{1}{4}(c_2-c_3)tx}}{[(c_2+c_3)-(c_2-c_3)x]\sqrt{2c_1-(c_2+c_3)+(c_2-c_3)x}} \frac{dx}{\sqrt{1-x^2}} + R(t) \tag{8}$$

where $c_i = \dfrac{\sigma_1^2 + \sigma_2^2 + \sigma_3^2}{\sigma_i^2}$ and

$$|r(t)|^2 < \frac{1}{2\pi} c_1 \left(\frac{c_2}{c_1-c_2}\right)\left(\frac{c_3}{c_1-c_3}\right) t^{-1} e^{-c_1 t}$$

$$|R(t)|^2 < \frac{2}{\pi c_1} \left(\frac{c_2}{c_1-c_2}\right)\left(\frac{c_3}{c_1-c_3}\right) t^{-1} e^{-c_1 t}$$

Two of the variances equal σ_j^2, third variance is $\sigma_i^2 \neq \sigma_j^2$

$$f(t) = \frac{1}{2} c_j \sqrt{\frac{c_i}{|c_i - c_j|}} \; e^{-\frac{c_j t}{2}} \; \mathrm{erf}\sqrt{\tfrac{1}{2}|c_i - c_j| t}$$

$$F(t) = I\left(\frac{1}{\sqrt{2}} c_i t, \; -\frac{1}{2}\right) - \sqrt{\frac{c_i}{|c_i - c_j|}} \; e^{-\frac{c_j t}{2}} \; \mathrm{erf}\sqrt{\tfrac{1}{2}|c_i - c_j| t}$$

where

$$\mathrm{erf}\, Z = \frac{2}{\sqrt{\pi}} \int_0^Z e^{-u^2} \, du$$

and $I(u,p)$ is the incomplete gamma function

$$\frac{1}{\Gamma(p+1)} \int_0^{u\sqrt{p+1}} e^{-t} \, t^p \, dt \quad .$$

3. Applications

The cumulative distribution of the magnitude of the mid-course velocity correction vector can be examined by applying the techniques of section 1. The mid-course velocity correction vector

$$\vec{\Delta V} = \begin{bmatrix} \Delta V_1 \\ \Delta V_2 \\ \Delta V_3 \end{bmatrix}$$

is assumed to be a 3-dimensional normal random vector with mean vector $\vec{0}^{1x3}$ and covariance matrix Σ. Consider an orthogonal transformation $P\vec{\Delta V}$ such that $P \Sigma P'$, the covariance matrix of the transformed vector, is diagonal, say

$$\begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{bmatrix}$$

The components of

$$P\overrightarrow{\Delta V} = \begin{bmatrix} \Delta V_1' \\ \Delta V_2' \\ \Delta V_3' \end{bmatrix}$$

are therefore mutually independent with variances σ_1^2, σ_2^2, σ_3^2 (the eigenvalues of $\sum$). Hence the method of section 1 may be applied to the distribution of $|P\overrightarrow{\Delta V}|^2 = (\Delta V_1')^2+(\Delta V_2')^2+(\Delta V_3')^2$. Because the magnitude of a vector is unaffected by orthogonal transformation, the distribution of $|P\overrightarrow{\Delta V}|^2$ is the same as that of $|\overrightarrow{\Delta V}|^2$.

It should be noted that unless there is a need to find the eigenvalues of $\sum$ for some other aspect of the study, it is not necessary to diagonalize $\sum$ in order to apply section 1. In equations (3) and (4) it is seen that σ^2 and ν are functions of $\sigma_1^2 + \sigma_2^2 + \sigma_3^2$ and $\sigma_1^4 + \sigma_2^4 + \sigma_3^4$, the traces of $P\sum P'$ and $(P\sum P')^2$, respectively. The trace is invariant under orthogonal transformation so that $\mathrm{tr}\sum = \mathrm{tr}(P\sum P') = \sigma_1^2 + \sigma_2^2 + \sigma_3^2$, and $\mathrm{tr}(\sum^2) = \mathrm{tr}(P\sum^2 P') = \mathrm{tr}(P\sum I\sum P') = \mathrm{tr}(P\sum P'P\sum P') = \mathrm{tr}(P\sum P')^2 = \sigma_1^4 + \sigma_2^4 + \sigma_3^4$. Thus equations (3) and (4) may be written

$$\sigma^2 = \mathrm{tr}(\textstyle\sum^2)/\mathrm{tr}\sum \tag{3'}$$

$$\nu = (\mathrm{tr}\textstyle\sum)^2/\mathrm{tr}(\sum^2) \quad . \tag{4'}$$

The table at the end of this section gives the results of cases in which the methods of sections 1 and 2 were applied to the mid-course velocity correction vector. In order to clarify the meaning of the results, the main steps involved in calculating the first line of the table are given below.

$$\vec{\Delta V} = \begin{bmatrix} \Delta V_1 \\ \Delta V_2 \\ \Delta V_3 \end{bmatrix}$$

is a normal random vector with mean vector $\vec{0}$ and covariance matrix

$$\Sigma = \begin{bmatrix} 5.3609 & -2.5262 & -4.7870 \\ -2.5262 & 1.3591 & 1.5323 \\ -4.7870 & 1.5323 & 7.4247 \end{bmatrix} \times 10^{-3}$$

$\vec{\Delta V}$ will be approximated by a $\sigma^2\chi_\nu^2$-variate where σ^2 and ν are found both by solving for the eigenvalues of Σ and by application of the properties of the trace. The eigenvalues of Σ are

$$\sigma_1^2 = 1.2021 \times 10^{-2} \quad , \quad \sigma_2^2 = 2.1222 \times 10^{-3} \quad , \quad \sigma_3^2 = 1.6453 \times 10^{-6}$$

By equations (3) and (4),

$$\sigma^2 = \frac{1.4901 \times 10^{-4}}{1.4145 \times 10^{-2}} = 1.0534 \times 10^{-2}$$

$$\nu = \frac{2.0008 \times 10^{-4}}{1.4901 \times 10^{-4}} = 1.3427$$

σ^2 and ν will now be found by using equations (3') and (4').

$$\Sigma^2 = \begin{bmatrix} 5.8037 & -2.4312 & -6.5076 \\ -2.4312 & 1.0577 & 2.5553 \\ -6.5076 & 2.5553 & 8.0390 \end{bmatrix} \times 10^{-5}$$

$$\mathrm{tr}\,\Sigma = 1.4145 \times 10^{-2}$$

$$\mathrm{tr}\,\Sigma^2 = 1.4900 \times 10^{-4}$$

Hence

$$\sigma^2 = \frac{1.4900 \times 10^{-4}}{1.4145 \times 10^{-2}} = 1.0534 \times 10^{-2}$$

$$\nu = \frac{2.0008 \times 10^{-4}}{1.4900 \times 10^{-4}} = 1.3428$$

For p = .90, $\zeta_p(\nu)$ must be found such that

$$P\left\{\sigma^2 \chi_\nu^2 \leq \zeta_p(\nu)\right\} = p \text{ or equivalently } P\left\{\chi_\nu^2 \leq \frac{\zeta_p(\nu)}{\sigma^2}\right\} = p.$$

Since ν is not an integer $\frac{\zeta_p(\nu)}{\sigma^2}$ will be found by 3-point interpolation. From a χ^2-table, the following is obtained.

$$P\{\chi_1^2 \leq 2.7055\} = .90$$

$$P\{\chi_2^2 \leq 4.6052\} = .90$$

$$P\{\chi_3^2 \leq 6.2514\} = .90$$

i.e.,

$$\frac{\zeta_{.90}(1)}{1.0534 \times 10^{-2}} = 2.7055 \quad , \quad \frac{\zeta_{.90}(2)}{1.0534 \times 10^{-2}} = 4.6052 \quad ,$$

$$\frac{\zeta_{.90}(3)}{1.0534 \times 10^{-2}} = 6.2514$$

Let

$$\frac{\zeta_p(\nu)}{\sigma^2} = a\nu^2 + b\nu + c$$

$$\nu = 1 : 2.7055 = a + b + c$$

$$\nu = 2 : 4.6052 = 4a + 2b + c$$

$$\nu = 3 : 6.2514 = 9a + 3b + c$$

Solving for the coefficients, one obtains

$$a = -0.1267 \quad , \quad b = 2.2797 \quad , \quad c = 0.5525$$

Hence

$$\frac{\zeta_{.90}(1.3427)}{1.0534 \times 10^{-2}} = (-0.1267)(1.3427)^2 + (2.2797)(1.3427) + (0.5525)$$

and

$$\zeta_{.90}(1.3427) = 3.5660 \times 10^{-2}$$

It should be emphasized that for any fixed probability level (here p = .90), the coefficients a, b, c of the polynomial used in the 3-point interpolation need only be solved for once. This same polynomial may be used for any ν and σ^2 at the same p level.

Under the assumption that $|\vec{\Delta V}|^2 = (\Delta V_1)^2 + (\Delta V_2)^2 + (\Delta V_3)^2$ can be approximated by a $\sigma^2\chi_\nu^2$-variate,

$$P\{(\Delta V_1)^2 + (\Delta V_2)^2 + (\Delta V_3)^2 \leq 3.5660 \times 10^{-2}\} \approx .90 \quad .$$

From section 2 the exact value of

$$P\{(\Delta V_1)^2 + (\Delta V_2)^2 + (\Delta V_3)^2 \leq 3.5660 \times 10^{-2}\}$$

is given by $G(3.5660 \times 10^{-2})$, the distribution function of $|\vec{\Delta V}|^2$ evaluated at 3.5660×10^{-2}. By equation (6),

$$G(t) = F\left(\frac{t}{\sum_1^3 \sigma_i^2}\right) \quad .$$

$$G(3.5660 \times 10^{-2}) = F(2.5211)$$

The integral in equation (8) was evaluated by means of the formula

$$\int_{-1}^{1} h(x) \frac{1}{\sqrt{1-x^2}} dx = \lim_{n\to\infty} \frac{\pi}{n} \sum_{i=1}^{n} h(x_i)$$

$$x_i = \cos \frac{(2i-1)\pi}{n}$$

See Abramowitz and Stegun [5], page 889 (25.4.38). For the examples considered here, $|R(t)|$ was negligible.

σ_1^2	σ_2^2	σ_3^2	p	ζ_p	$G(\zeta_p)$
1.2021×10^{-2}	2.1222×10^{-3}	1.6453×10^{-6}	.90	3.5660×10^{-2}	.9035
			.95	4.8616×10^{-2}	.9501
			.99	7.9717×10^{-2}	.9888
			.995	9.3378×10^{-2}	.9941
			.999	1.2550×10^{-1}	.9986
2.0346×10^{1}	5.5297	1.3739×10^{-1}	.90	6.3729×10^{1}	.9045
			.95	8.5532×10^{1}	.9506
			.99	1.3732×10^{2}	.9887
			.995	1.5992×10^{2}	.9939
			.999	2.1286×10^{2}	.9985
5.9302×10^{-1}	2.3123×10^{-1}	7.7983×10^{-3}	.90	1.9858	.9042
			.95	2.6290	.9509
			.99	4.1421	.9889
			.995	4.7987	.9940
			.999	6.3314	.9986
6.0922×10^{-1}	2.2815×10^{-1}	2.5941×10^{-2}	.90	2.0470	.9049
			.95	2.7013	.9509
			.99	4.2365	.9887
			.995	4.9018	.9939
			.999	6.4531	.9985

CONCLUSIONS

A comparison of p and $G(\zeta_p)$ in the table indicates that ζ_p is an excellent approximation of the quantile of order p. There is very little variation in the accuracy of ζ_p for the widely differing triplets of eigenvalues of Σ. The accuracy and ease in applying the methods of section 1 make it desirable for examining the distribution functions of quadratic forms such as $|\overrightarrow{\Delta V}|^2$.

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Attachment
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